

# Quantum correlations in different density matrix representations of spin-1/2 open chain

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## Abstract

We consider quantum correlations in a spin-1/2 open chain of  $N$  nodes with the XY Hamiltonian using different bases for the density matrix representation and the initial state with a single polarized node. These bases of our choice are following: (i) the basis of eigenvectors of the fermion operators; this basis appears naturally through the Jordan-Wigner transformation (this representation of the density matrix is referred to as the  $\beta$ -representation), (ii) its Fourier representation ( $c$ -representation of the density matrix) and (iii) the basis of eigenvectors of the operators  $I_{jz}$  (the  $z$ -projection of the  $j$ th spin,  $j = 1, \dots, N$ ). Although for the short chains (a few nodes) the qualitative behavior of the entanglement and the discord are very similar (the difference is quantitative), this is not valid for longer chains ( $N \gtrsim 10$ ). In this case, there are qualitative and quantitative distinctions between the entanglement and the discord in all three cases. We underline three most important features: (i) the quantum discord is static in the  $\beta$ -representation, where the entanglement is identical to zero; (ii) in the  $c$ -representation, the concurrence may be non-zero only between the nearest neighbors (with a single exception), while the discord is nonzero between any two nodes; (iii) there is so-called "echo" in the evolution of the discord, which is not observed in the evolution of the concurrence. Using different bases, we may choose the preferable behavior of quantum correlations which allows a given quantum system to be more flexible in applications.

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## I. INTRODUCTION

The advantage of quantum correlations in comparison with classical ones rises a fast development of quantum information and communication devices. However, the problem of identifying of quantum correlations in a given system is not resolved yet. First, the so-called quantum entanglement [1–5] was considered as a proper measure of quantum correlations. Later on, the quantum discord was accepted as a more adequate measure of quantum correlations [6–9]. In particular, the states with zero entanglement can reveal non-zero discord. Therefore it was noted [10] that namely discord might be responsible for advantages of quantum information devices, in particular, for quantum speed-up. In general, the calculation of discord is very cumbersome optimization problem. In spite of intensive study of discord only very special cases have been treated analytically [11–13]. Nevertheless, namely these cases correspond to the reduced binary density matrix in spin-1/2 chains governed by different Hamiltonians with either the thermal equilibrium initial state [14, 15] or the initial state with a single polarized node.

A problem of a proper initial state is one of the fundamental problems in study of quantum correlations in different physical systems because of the technical difficulties of realization of a particular state. Most popular is so-called thermal equilibrium initial state [14], which is most simple for realization. However, the initial state with a single excited node is more relative, for instance, in quantum communication lines [16–21]. The state with a single polarized node has been produced experimentally [22]. The evolution of quantum systems with this initial state at high temperatures has been studied, for instance, in [23], where the quantum echo has been found.

Nevertheless, the problem of identification of quantum correlations is not resolved yet. In particular, the measure of quantum correlations depends on the basis which is taken for the density matrix representation. The reason is that, considering different bases, we involve different types of "virtual particles". A possible way to avoid this ambiguity is suggested in ref.[24], where the unitary invariant discord is introduced. This measure takes into account correlations among all possible "virtual particles".

In this paper we consider the problem of preferable "virtual particles" (or the preferable basis of the matrix representation) from a different viewpoint. Instead of collecting the correlations among all "virtual particles" (like in the unitary invariant discord [24]) we con-

sider separately the quantum correlations among three types of particles, namely, among the fermions, which appear in a spin-1/2 system with the nearest neighbor interaction under the Jourdan-Wigner transformation [25] (we call them as the  $\beta$ -fermions), among the fermions which are the Fourier representations of the  $\beta$ -fermions (the  $c$ -fermions), and among the spin-1/2 particles in the basis of eigenvectors of the operators  $I_{jz}$  ( $z$ -projection of the  $j$ th spin,  $j = 1, \dots, N$ ). Each type of particles corresponds to the proper basis of the density matrix representation. We show, that the choice of the basis is a significant (may be even dominant) factor in identification of quantum correlations.

This paper is organized as follows. The evolution of the spin-1/2 open chain of  $N$  nodes under the XY Hamiltonian with the nearest neighbor interactions is derived in Sec.II using the Jourdan-Wigner transformation. The general formulas for the discord and the concurrence are discussed in Sec.III. The comparison of the discord and the concurrence in different bases of the density matrix representation is given in Sec.IV. The summary of our results is represented in Sec.V.

## II. SPIN-1/2 CHAINS WITH A SINGLE INITIALLY POLARIZED NODE

In this paper we study the quantum correlations in the one-dimensional open spin-1/2 chain of  $N$  nodes governed by the XY Hamiltonian in the approximation of nearest neighbor interactions,

$$H = \omega_0 \sum_{i=1}^N I_{iz} + D \sum_{i=1}^{N-1} (I_{ix}I_{(i+1)x} + I_{iy}I_{(i+1)y}), \quad (1)$$

where  $\omega_0$  is the Larmour frequency in the external magnetic field,  $D$  is the spin-spin coupling constant between the nearest neighbors and  $I_{i\alpha}$  ( $i = 1, \dots, N$ ,  $\alpha = x, y, z$ ) is the  $i$ th spin projection on the  $\alpha$ -axis. We chose the initial state of this chain with the single polarized  $j$ th node ( $1 \leq j \leq N$ ) at arbitrary temperature, i.e.

$$\rho_0 = \frac{e^{\beta I_{jz}}}{Z} = \frac{1}{2^N} \left( 1 + 2I_{jz} \tanh \frac{\beta}{2} \right), \quad Z = \text{Tr}(e^{\beta I_{jz}}) = 2^N \cosh \frac{\beta}{2}, \quad (2)$$

where  $\beta = \frac{\hbar\omega_0}{kT}$ ,  $\hbar$  is the Plank constant,  $k$  is the Boltzmann constant, and  $T$  is the temperature of the system. The evolution of the density matrix is described by the Liouville equation  $\frac{d\rho}{dt} = -i[H, \rho]$  for the density matrix  $\rho$ . The solution to this equation reads:

$$\rho(t) = e^{-itH} \rho_0 e^{itH} = \frac{1}{2^N} e^{-iHt} (1 + 2I_{jz} \tanh \frac{\beta}{2}) e^{iHt}. \quad (3)$$

To solve the Liouville equation, we diagonalize the Hamiltonian (1) using the Jordan-Wigner transformation method [25]

$$H = \sum_k \varepsilon_k \beta_k^+ \beta_k - \frac{1}{2} N \omega_0, \quad \varepsilon_k = D \cos(k) + \omega_0, \quad (4)$$

where the fermion operators  $\beta_j$  are defined in terms of other fermion operators  $c_j$  by means of the Fourier transformation

$$\beta_k = \sum_{j=1}^N g_k(j) c_j, \quad (5)$$

and the fermion operators  $c_j$  are defined as [25]

$$c_j = (-2)^{j-1} I_{1z} I_{2z} \dots I_{z(j-1)} I_j^-. \quad (6)$$

Here

$$g_k(j) = \left( \frac{2}{N+1} \right)^{1/2} \sin(kj), \quad k = \frac{\pi n}{N+1}, \quad n = 1, 2, \dots, N. \quad (7)$$

It may be readily shown that the projection operators  $I_{jz}$  can be expressed in terms of the fermion operators  $c_j$  as

$$I_{jz} = c_j^+ c_j - \frac{1}{2}, \quad \forall j. \quad (8)$$

Then the density matrix (3) can be transformed to the following form [23]

$$\rho(t) = \frac{1 - \tanh \frac{\beta}{2}}{2^N} + \frac{\tanh \frac{\beta}{2}}{2^{N-1}} \sum_{k,k'} e^{-it(\varepsilon_k - \varepsilon_{k'})} g_k(j) g_{k'}(j) \beta_k^+ \beta_{k'}. \quad (9)$$

where we use the identity

$$e^{-i\varphi \beta_k^+ \beta_k} \beta_k^+ e^{i\varphi \beta_k^+ \beta_k} = e^{-i\varphi} \beta_k^+, \quad \forall \varphi. \quad (10)$$

It is interesting to note that the quantity  $\frac{\langle I_{pz} \rangle(t)}{\langle I_{jz} \rangle(0)}$  for the  $p$ th node does not depend on  $\beta$  and coincides with the result of ref.[23] obtained for the high temperatures only ( $\langle a \rangle \equiv \text{Tr}\{\rho a\}$  for any operator  $a$ ):

$$\frac{\langle I_{pz} \rangle(t)}{\langle I_{jz} \rangle(0)} = \frac{4}{(N+1)^2} \left| \sum_k e^{-i\varepsilon_k t} \sin(kj) \sin(kp) \right|^2. \quad (11)$$

We will study the quantum discord  $Q_{nm}$  and the concurrence  $C_{nm}$  (as a measure of entanglement) between any two particles. Since  $Q_{nm} = Q_{mn}$  and  $C_{nm} = C_{mn}$ , hereafter we

take  $m > n$  without loss of generality,  $n = 1, \dots, N$ . As was mentioned in the Introduction, we consider the open spin-1/2 chain using its density matrix representations in three different bases: (i) the basis of eigenvectors of the fermion operators  $\beta_j$  (we refer to this representation of the density matrix as the  $\beta$ -representation), (ii) the basis of eigenvectors of the Fourier transformed fermion operators  $c_j$  (the  $c$ -representation of the density matrix), and (iii) the basis of eigenvectors of the operators  $I_{jz}$  ( $j = 1, \dots, N$ ). Of course, considering the correlations between the  $n$ th and the  $m$ th nodes in all these cases we consider the quantum correlations between physically different particles. Thus, using either the  $\beta$ - or  $c$ -representation we consider the correlations either between the  $n$ th and  $m$ th  $\beta$ -fermions or between the  $n$ th and  $m$ th  $c$ -fermions, while using the basis of eigenvectors of the operators  $I_{jz}$ , we elaborate quantum correlations between the natural spin-1/2 particles. This is the reason of qualitative and quantitative difference among the discords and entanglements found in all these cases.

First step in calculation of either discord or entanglement between the  $n$ th and  $m$ th nodes is the construction of the reduced density matrix with respect to all nodes except for the  $n$ th and  $m$ th ones. Below, we calculate the reduced density matrices in three different bases mentioned above. In all cases we use notations

$$|nm\rangle = \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\} \quad (12)$$

for the basis vectors, where  $n$  in the vector  $|n\rangle$  means the different filling numbers in the fermion bases or the excited spin ( $n = 1$ ) and the ground state spin ( $n = 0$ ) in the basis of eigenvectors of operators  $I_{jz}$ .

#### A. The reduced density matrix in the basis of eigenvectors of the fermion operators $\beta_j$

We use the superscript " $\beta$ " to specify the  $\beta$ -representations of quantum operators. Let us reduce density matrix (9) with respect to all fermions except for the  $n$ th and  $m$ th ones obtaining:

$$\rho_{nm}^{\beta} = \frac{1}{4} - \frac{\tanh \frac{\beta}{2}}{4} (g_n^2(j) + g_m^2(j)) + \frac{\tanh \frac{\beta}{2}}{2} \sum_{k, k'=n, m} e^{-it(\varepsilon_k - \varepsilon_{k'})} g_k(j) g_{k'}(j) \beta_k^+ \beta_{k'}. \quad (13)$$

Using the basis (12) we find

$$\rho_{nm}^\beta = \begin{pmatrix} J_{00}^\beta + J_{mm}^\beta + J_{nn}^\beta & 0 & 0 & 0 \\ 0 & J_{00}^\beta + J_{mm}^\beta & J_{mn}^\beta & 0 \\ 0 & J_{nm}^\beta & J_{00}^\beta + J_{nn}^\beta & 0 \\ 0 & 0 & 0 & J_{00}^\beta \end{pmatrix}, \quad (14)$$

where

$$\begin{aligned} J_{00}^\beta &= \frac{1}{4} - \frac{\tanh \frac{\beta}{2}}{4} (g_n^2(j) + g_m^2(j)), \\ J_{nm}^\beta &= \frac{\tanh \frac{\beta}{2}}{2} e^{-it(\varepsilon_n - \varepsilon_m)} g_n(j) g_m(j) \end{aligned} \quad (15)$$

It is obvious that

$$J_{nn}^\beta = \frac{\tanh \frac{\beta}{2}}{2} g_n^2(j), \quad (16)$$

which does not depend on the time  $t$ .

## B. The reduced density matrix in the basis of eigenvectors of the fermion operators $c_j$

In this case we write the density matrix (9) as

$$\rho(t) = \frac{1 - \tanh \frac{\beta}{2}}{2^N} + \frac{\tanh \frac{\beta}{2}}{2^{N-1}} \sum_{k,k',l,l'} e^{-it(\varepsilon_k - \varepsilon_{k'})} g_k(j) g_{k'}(j) g_k(l) g_{k'}(l') c_l^+ c_{l'}. \quad (17)$$

We use the superscript "c" to specify the  $c$ -representations of quantum operators. Reducing the density matrix  $\rho$  with respect to all fermions except for the  $n$ th and  $m$ th ones, we obtain

$$\begin{aligned} \rho_{nm}^c &= \frac{1}{4} - \frac{\tanh \frac{\beta}{2}}{4} \sum_{k,k'} \sum_{l=n,m} e^{-it(\varepsilon_k - \varepsilon_{k'})} g_k(j) g_{k'}(j) g_k(l) g_{k'}(l) + \\ &\frac{\tanh \frac{\beta}{2}}{2} \sum_{k,k'} \sum_{l,l'=n,m} e^{-it(\varepsilon_k - \varepsilon_{k'})} g_k(j) g_{k'}(j) g_k(l) g_{k'}(l') c_l^+ c_{l'}. \end{aligned} \quad (18)$$

The matrix form of the reduced density matrix  $\rho_{nm}^c$  in the basis (12) coincides with eq.(14) up to the replacements  $J_{nm}^\beta \rightarrow J_{nm}^c$  with

$$\begin{aligned} J_{00}^c &= \frac{1}{4} - \frac{\tanh \frac{\beta}{2}}{4} \sum_{k,k'} \sum_{l=n,m} e^{-it(\varepsilon_k - \varepsilon_{k'})} g_k(j) g_{k'}(j) g_k(l) g_{k'}(l) = \\ &\quad \frac{1}{4} - \frac{1}{2} (J_{nn}^c + J_{mm}^c), \\ J_{nm}^c &= \frac{\tanh \frac{\beta}{2}}{2} \sum_{k,k'} e^{-it(\varepsilon_k - \varepsilon_{k'})} g_k(j) g_{k'}(j) g_k(n) g_{k'}(m). \end{aligned} \quad (19)$$

It is obvious that

$$J_{nn}^c(t) = \frac{\tanh \frac{\beta}{2}}{2} \left| \sum_k e^{-it\varepsilon_k} g_k(j) g_k(n) \right|^2, \quad J_{nn}^c(0) = \frac{\tanh \frac{\beta}{2}}{2} \delta_{jn}, \quad (20)$$

where  $\delta_{jn}$  is the Kronecker symbol. Eq.(20) means, in particular, that  $J_{nn}^c \leq \frac{1}{2}$ .

### C. The reduced density matrix in the basis of eigenvalues of operators $I_{jz}$ , $j = 1, \dots, N$

In this case we write the density matrix as

$$\begin{aligned} \rho(t) &= \frac{1 - \tanh \frac{\beta}{2}}{2^N} + \frac{\tanh \frac{\beta}{2}}{2^{N-1}} \sum_{k,k',l,l'} e^{-it(\varepsilon_k - \varepsilon_{k'})} g_k(j) g_{k'}(j) g_k(l) g_{k'}(l') \times \\ &\quad (-2)^{l+l'-2} I_{1z} \dots I_{(l-1)z} I_l^+ I_{1z} \dots I_{(l'-1)z} I_{l'}^-. \end{aligned} \quad (21)$$

We use the superscript "spin" to specify the matrix representations of quantum operators in the basis of eigenvectors of the operators  $I_{jz}$ . Reducing the density matrix  $\rho$  with respect to all nodes except for the  $n$ th and  $m$ th ones, we obtain that the reduced density matrix is non-diagonal only if  $m = n \pm 1$ :

$$\begin{aligned} \rho_{n(n+1)}^{spin} &= \frac{1}{4} - \frac{\tanh \frac{\beta}{2}}{4} \sum_{k,k'} \sum_{l=n,n+1} e^{-it(\varepsilon_k - \varepsilon_{k'})} g_k(j) g_{k'}(j) g_k(l) g_{k'}(l) + \\ &\quad \frac{\tanh \frac{\beta}{2}}{2} \sum_{k,k'} e^{-it(\varepsilon_k - \varepsilon_{k'})} g_k(j) g_{k'}(j) \left( g_k(n) g_{k'}(n+1) I_n^+ I_{n+1}^- + g_k(n+1) g_{k'}(n) I_{n+1}^+ I_n^- + \right. \\ &\quad \left. g_k(n) g_{k'}(n) I_n^+ I_n^- + g_k(n+1) g_{k'}(n+1) I_{n+1}^+ I_{n+1}^- \right) \end{aligned} \quad (22)$$

Otherwise ( $m \neq n \pm 1$ ) the density matrix is diagonal:

$$\begin{aligned} \rho_{nm}^{spin} = & \frac{1}{4} - \frac{\tanh \frac{\beta}{2}}{4} \sum_{k,k'} \sum_{l=n,m} e^{-it(\varepsilon_k - \varepsilon_{k'})} g_k(j) g_{k'}(j) g_k(l) g_{k'}(l) + \\ & \frac{\tanh \frac{\beta}{2}}{2} \sum_{k,k'} e^{-it(\varepsilon_k - \varepsilon_{k'})} g_k(j) g_{k'}(j) \left( g_k(n) g_{k'}(n) I_n^+ I_n^- + g_k(m) g_{k'}(m) I_m^+ I_m^- \right), \end{aligned} \quad (23)$$

so that the discord and entanglement are both zero. The matrix form of the reduced density matrix  $\rho_{n(n+1)}^{spin}$  in the basis (12) coincides with eq.(14) up to the replacements  $J_{nm}^\beta \rightarrow J_{nm}^{spin}$  with

$$J_{00}^{spin} = J_{00}^c, \quad J_{nn}^{spin} = J_{nn}^c, \quad J_{(n+1)(n+1)}^{spin} = J_{(n+1)(n+1)}^c, \quad J_{n(n+1)}^{spin} = J_{n(n+1)}^c. \quad (24)$$

### III. GENERAL FORMULAS FOR DISCORD AND CONCURRENCE

Since the reduced bi-particle density matrices in all three cases have the same matrix form (14), we derive the formulas for both the concurrence (as a measure of entanglement) and the discord for the density matrix (14) omitting the superscript  $\beta$ . We will use the relation

$$|J_{mn}|^2 = J_{nn} J_{mm} \quad (25)$$

which is valid in all three cases considered in Secs.II A-II C.

#### A. Concurrence

We characterize the entanglement by the Wootters criterion in terms of the concurrence [26, 27]. According to [26, 27], one needs to construct the spin-flip density matrix

$$\tilde{\rho}_{(nm)}(\tau) = (\sigma_y \otimes \sigma_y) (\rho^{(nm)})^*(\tau) (\sigma_y \otimes \sigma_y), \quad (26)$$

where the asterisk denotes the complex conjugation in the basis (12) and the Pauli matrix  $\sigma_y = 2I_y$ . The concurrence for the density matrix  $\rho_{(nm)}(\tau)$  is equal to

$$C = \max(0, 2\lambda - \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4), \quad \lambda = \max(\lambda_1, \lambda_2, \lambda_3, \lambda_4), \quad (27)$$



where  $\lambda_1, \lambda_2, \lambda_3$  and  $\lambda_4$  are the square roots of the eigenvalues of the matrix product  $\rho_{(nm)}(\tau)\tilde{\rho}_{(nm)}(\tau)$ . For the density matrix  $\rho$  given by eq.(14) we have

$$\begin{aligned}\lambda &= \lambda_1 = \frac{1}{4}\sqrt{1 - 4(J_{mm} - J_{nn})^2} + \sqrt{J_{mm}J_{nn}}, \\ \lambda_2 &= \frac{1}{4}\sqrt{1 - 4(J_{mm} - J_{nn})^2} - \sqrt{J_{mm}J_{nn}}, \\ \lambda_3 &= \lambda_4 = \frac{1}{4}\sqrt{1 - 4(J_{mm} + J_{nn})^2}.\end{aligned}\tag{28}$$

Substituting eqs.(28) into eq.(27) we obtain

$$C_{nm} = \max \left( 0, 2\sqrt{J_{mm}J_{nn}} - \frac{1}{2}\sqrt{1 - 4(J_{mm} + J_{nn})^2} \right).\tag{29}$$

## B. Discord

As far as matrix (14) is a particular case of the X-matrix, we will use the results of ref. [12], where the discord for the X-matrix has been studied. We remind the basic formulas for calculation of the discord  $Q^{(B)}$  between two particles, which are called the subsystems  $A$  and  $B$  [12]. Recall, that the superscript  $B$  means that the projective measurements are performed over the subsystem  $B$ . The discord is introduced as a difference between the total mutual information  $I(\rho)$  encoded into the system  $AB$  and its classical part  $\mathcal{C}^B$ ,

$$Q^{(B)} = I(\rho) - \mathcal{C}^{(B)},\tag{30}$$

The total mutual information  $I$  reads

$$I(\rho) = S(\rho^{(A)}) + S(\rho^{(B)}) + \sum_{j=0}^3 \lambda_j \log_2 \lambda_j.\tag{31}$$

Here  $\rho^{(A)}$  and  $\rho^{(B)}$  of the reduced density matrices of the subsystems  $A$  and  $B$ ,  $S(\rho^{(A)})$  and  $S(\rho^{(B)})$  are the von Neumann entropies of the subsystems  $A$  and  $B$ ,

$$\begin{aligned}S(\rho^{(A)}) &= -\frac{1}{2} \left( \log_2 \left( \frac{1}{4} - J_{mm}^2 \right) + 2J_{mm} \log_2 \frac{1 + 2J_{mm}}{1 - 2J_{mm}} \right), \\ S(\rho^{(B)}) &= -\frac{1}{2} \left( \log_2 \left( \frac{1}{4} - J_{nn}^2 \right) + 2J_{nn} \log_2 \frac{1 + 2J_{nn}}{1 - 2J_{nn}} \right),\end{aligned}\tag{32}$$

$\lambda_j$  are the eigenvalues of the density matrix (14),

$$\lambda_{0,1} = \frac{1}{4}(1 - 2(J_{mm} + J_{nn})), \quad \lambda_{2,3} = \frac{1}{4}(1 + 2(J_{mm} + J_{nn})).\tag{33}$$

As far as all eigenvalues of any density matrix must be non-negative, eqs.(33) mean

$$J_{mm} + J_{nn} \leq 1/2. \quad (34)$$

The classical counterpart  $\mathcal{C}^{(B)}$  reads [12]

$$\mathcal{C}^{(B)} = S(\rho^{(A)}) - \min_{\eta=\{0,1\}} (p_0 S_0 + p_1 S_1). \quad (35)$$

Here the conditional entropies  $S_i$  ( $i = 0, 1$ ) are

$$\begin{aligned} S_i &= -\frac{1 - \theta^{(i)}}{2} \log_2 \frac{1 - \theta^{(i)}}{2} - \frac{1 + \theta^{(i)}}{2} \log_2 \frac{1 + \theta^{(i)}}{2}, \\ \theta^{(0)} &= \frac{2\sqrt{J_{mm}(J_{mm} - (\eta^2 - 1)J_{nn})}}{1 + 2\eta J_{nn}}, \quad \theta^{(1)} = \frac{2\sqrt{J_{mm}(J_{mm} - (\eta^2 - 1)J_{nn})}}{1 - 2\eta J_{nn}} \end{aligned} \quad (36)$$

and the populations  $p_i$ ,  $i = 0, 1$  are

$$p_0 = \frac{1}{2}(1 + 2\eta J_{nn}), \quad p_1 = \frac{1}{2}(1 - 2\eta J_{nn}), \quad (37)$$

where we introduce the parameter  $\eta$  instead of  $k$  used in ref.[12],  $k = \frac{1+\eta}{2}$ . It might be readily demonstrated that the minimum in eq.(35) corresponds to  $\eta = 0$ . For this purpose we show that the derivative of the function

$$f(\eta) = p_0 S_0 + p_1 S_1 \quad (38)$$

with respect to the parameter  $\eta$  is positive over the interval  $0 \leq \eta \leq 1$ . In fact, this derivative reads after some transformations:

$$\begin{aligned} f'(\eta) &= (\alpha + \beta) \log_2 \frac{1 - 2\eta J_{nn} + 2d}{1 + 2\eta J_{nn} - 2d} + \\ &(\beta - \alpha) \log_2 \frac{1 + 2\eta J_{nn} + 2d}{1 - 2\eta J_{nn} - 2d} + 2\alpha \log_2 \frac{1 + 2\eta J_{nn}}{1 - 2\eta J_{nn}}, \\ \alpha &= \frac{J_{nn}}{2}, \quad \beta = \frac{\eta J_{mm} J_{nn}}{2d}, \quad d = \sqrt{J_{mm}(J_{mm} - (\eta^2 - 1)J_{nn})}. \end{aligned} \quad (39)$$

Collecting terms with  $\alpha$  and  $\beta$  we obtain:

$$f'(\eta) = \alpha \log_2 \frac{4d^2(1 + 2\eta J_{nn})^2 - (1 - 4\eta^2 J_{nn}^2)^2}{4d^2(1 - 2\eta J_{nn})^2 - (1 - 4\eta^2 J_{nn}^2)^2} + \beta \log_2 \frac{(1 + 2d)^2 - 4\eta^2 J_{nn}^2}{(1 - 2d)^2 - 4\eta^2 J_{nn}^2}. \quad (40)$$

Both terms in the RHS of eq.(40) are nonnegative. Thus we conclude that  $f'(\eta) \geq 0$ , i.e.  $f(\eta)$  is increasing function over the interval  $0 \leq \eta \leq 1$ . Consequently, the function  $f(\eta)$  takes the minimal value at the boundary point  $\eta = 0$ .

As a result, the expression for the classical correlations (35) reads:

$$\begin{aligned} \mathcal{C}^{(B)} = & \frac{1}{2} \log_2 \frac{1 - 4J_{mm}(J_{mm} + J_{nn})}{1 - 4J_{mm}^2} + J_{mm} \log_2 \frac{1 - 2J_{mm}}{1 + 2J_{mm}} + \\ & \sqrt{J_{mm}(J_{mm} + J_{nn})} \log_2 \frac{1 + 2\sqrt{J_{mm}(J_{mm} + J_{nn})}}{1 - 2\sqrt{J_{mm}(J_{mm} + J_{nn})}} \end{aligned} \quad (41)$$

Now the discord  $Q^{(B)}$  may be calculated by formula (30) using eqs.(31-33) and (41):

$$\begin{aligned} Q^{(B)} = & -\frac{1}{2} \left( (1 - 2J_{nn}) \log_2(1 - 2J_{nn}) + (1 + 2J_{nn}) \log_2(1 + 2J_{nn}) - \right. \\ & (1 - 2J_{mm} - 2J_{nn}) \log_2(1 - 2J_{mm} - 2J_{nn}) - \\ & (1 + 2J_{mm} + 2J_{nn}) \log_2(1 + 2J_{mm} + 2J_{nn}) + \\ & (1 - 2\sqrt{J_{mm}(J_{mm} + J_{nn})}) \log_2(1 - 2\sqrt{J_{mm}(J_{mm} + J_{nn})}) + \\ & \left. (1 + 2\sqrt{J_{mm}(J_{mm} + J_{nn})}) \log_2(1 + 2\sqrt{J_{mm}(J_{mm} + J_{nn})}) \right). \end{aligned} \quad (42)$$

Note that the discord  $Q^{(A)}$  (obtained by means of the Neumann type measurements over the subsystem  $A$ ) differs from the discord  $Q^{(B)}$  by the replacement  $n \leftrightarrow m$ . As far as  $Q^{(A)} \neq Q^{(B)}$  in general [7, 8], we define the discord  $Q_{nm}$  as follows [28]:

$$Q_{nm} = \min(Q_{nm}^{(A)}, Q_{nm}^{(B)}). \quad (43)$$

#### IV. DISCORD AND CONCURRENCE IN DIFFERENT DENSITY MATRIX REPRESENTATIONS OF THE OPEN SPIN CHAIN WITH $N \gtrsim 10$ NODES

The problem of description of those quantum correlations which are responsible for advantages of quantum computations is not resolved yet. Therefore it is reasonable to characterize different types of quantum correlations in a quantum system, i.e. not only those which correspond to the real particles, but also correlations between the "virtual particles". This was the basic motivation for introduction of the unitary invariant discord in ref.[24] as a way to count all quantum correlations between all possible "virtual particles". The geometric measure  $Q^G$  of the unitary invariant discord is representable in terms of eigenvalues  $\lambda_i$  of the considered density matrix,

$$Q^G = \frac{2^N \sum_{i=1}^{2^N} \lambda_i^2 - 1}{2^N - 1}, \quad (44)$$

so that it achieves the maximal value 1 for a pure state and is zero for the matrix with all equal eigenvalues. In the case of bi-particle density matrix (14),  $N = 2$ , with eigenvalues

(33) we obtain

$$Q_{nm}^G = \frac{4}{3}(J_{mm} + J_{nn})^2 \leq \frac{1}{3}. \quad (45)$$

The significant value of  $Q^G$  suggests us to look for such basis where the quantum correlations are valuable and/or the evolution of quantum correlations is suitable for applications.

In the present paper we investigate the quantum correlations in a spin-1/2 chain of  $N$  nodes using three different matrix representations, i.e. we consider the same chain using (i) the  $\beta$ -representation introduced in Sec.II A, (ii) the  $c$ -representation introduced in Sec.II B, and (iii) the representation in the basis of eigenvectors of the operators  $I_{jz}$ ,  $j = 1, \dots, N$ , discussed in Sec.II C. Below we study the quantum correlations in all three bases and demonstrate the significant qualitative and quantitative distinctions among the discord and the concurrence in all three cases. It will be illustrated that the discord in the  $\beta$ - and  $c$ -representations of the density matrix reveals the new properties of the considered quantum system in comparison with the usual discord in the basis of eigenvectors of the operators  $I_{jz}$ .

### A. Discord and concurrence in a system of $\beta$ -fermions

First, we consider the  $\beta$ -representation of the density matrix (see Sec.II A) and calculate the discord and the concurrence between the  $n$ th and  $m$ th fermions. Formula (27) for the concurrence reads in this case:

$$C_{nm}^\beta = \max \left( 0, \tanh \frac{\beta}{2} g_m(j) g_n(j) - \frac{1}{2} \sqrt{1 - \tanh^2 \frac{\beta}{2} (g_m^2(j) + g_n^2(j))^2} \right). \quad (46)$$

Simple estimation at  $\beta \rightarrow \infty$  shows that the concurrence may be positive only for  $N \leq 4$ , which is not interesting for us. In the case of longer chain,  $C_{nm}^\beta = 0$  for any nodes  $n$  and  $m$ .

The behavior of the discord is completely different. Using formulas (42) and (15) we obtain that the discord is non-zero in general and does not evolve in time. The discord  $Q_{n,n+1}$  between the nearest neighbors versus  $\beta = \frac{\hbar\omega_0}{kT}$  for  $N = 21$  is depicted in Fig.1. Emphasize that the discord is non-zero not only between the nearest neighbors, but between the remote nodes as well, which is not valid in general, see, for instance, Sec.IV C. The dependence of the discord  $Q_{n,n+l}^\beta$ ,  $l = 1, 2, 3, 4$ , on  $n$  for  $N = 21$  and large values of  $\beta$  ( $\beta = 10$ ) is shown in Fig.2 for different initially polarized nodes  $j = 1, 6, 10, 11$ . Fig.2 reveals the interesting properties of discord.

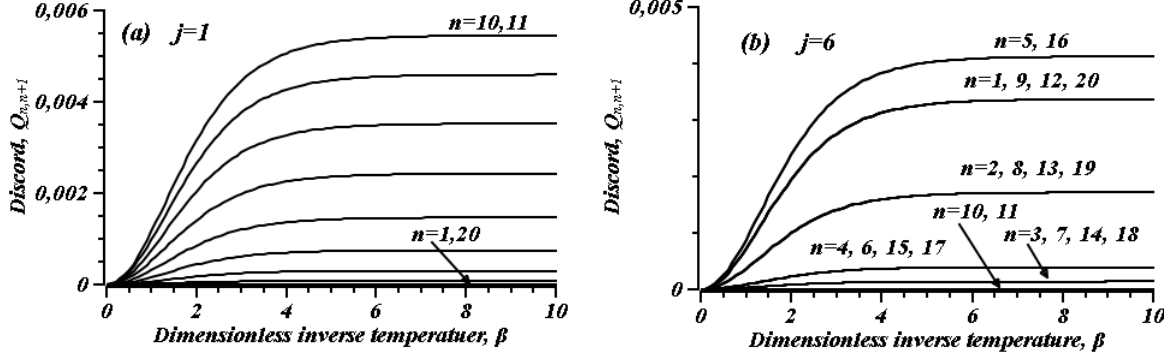


FIG. 1: The discord  $Q_{n,n+1}^\beta$  versus the dimensionless inverse temperature  $\beta$  for the spin chain with  $N = 21$ ; (a) the 1st node is initially polarized ( $j = 1$ ), the discord increases from the ends to the center of the chain; (b) the 6th node is initially polarized ( $j = 6$ ), the discord is a periodic function of the node  $n$ .

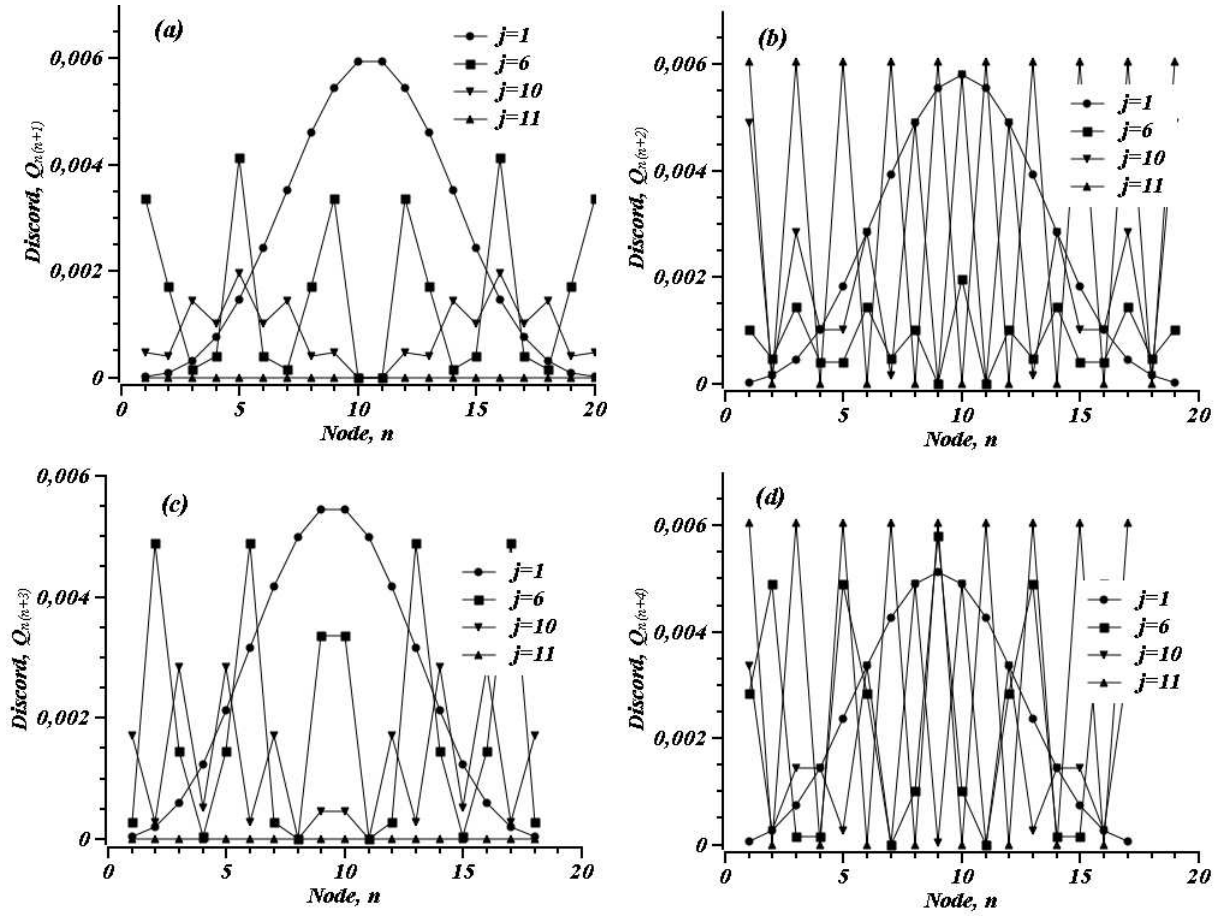


FIG. 2: The discord  $Q_{n,n+l}^\beta$ ,  $l = 1, 2, 3, 4$ , versus the node  $n$  for the chain of  $N = 21$  nodes and different initially polarized nodes  $j = 1, 6, 10, 11$

1. The discord possesses the following symmetry  $Q_{n,n+k}^\beta = Q_{N-n,N-n+k}^\beta$ , which is a consequence of the equality

$$g_{\frac{\pi n}{N+1}}(j) = g_{\frac{\pi(N+1-n)}{N+1}}(j) \quad (47)$$

and definition (43).

2. If  $N$  is odd and the middle node is initially polarized (i.e.  $j = \frac{N+1}{2}$ ), then the discord  $Q_{n,n+2k+1}^\beta$ ,  $k = 0, 1, \dots$  is zero, while the discord  $Q_{n,n+2k}^\beta$ ,  $k = 1, \dots$  is zero only for even  $n$ , namely

$$Q_{n,n+2k}^\beta = \begin{cases} 0, & n = 2i, \quad i = 1, 2, \dots \\ q, & n = 2i + 1, \quad i = 0, 1, \dots \end{cases} \quad k = 1, 2, \dots \quad (48)$$

$$q = \frac{1}{2} \log_2 \frac{\left( (N+1)^2 - \left( 4 \tanh \frac{\beta}{2} \right)^2 \right) (N+1)^2}{\left( (N+1)^2 - \left( 2 \tanh \frac{\beta}{2} \right)^2 \right) \left( (N+1)^2 - 2 \left( 2 \tanh \frac{\beta}{2} \right)^2 \right)} +$$

$$\frac{\tanh \frac{\beta}{2}}{N+1} \log_2 \frac{(N+1 + 4 \tanh \frac{\beta}{2})^2 (N+1 - 2 \tanh \frac{\beta}{2})}{(N+1 - 4 \tanh \frac{\beta}{2})^2 (N+1 + 2 \tanh \frac{\beta}{2})} +$$

$$\frac{\sqrt{2} \tanh \frac{\beta}{2}}{N+1} \log_2 \frac{(N+1 - 2\sqrt{2} \tanh \frac{\beta}{2})}{(N+1 + 2\sqrt{2} \tanh \frac{\beta}{2})}.$$

Here  $q$  depends only on  $\beta$  and  $N$  and does not depend on the particular choice of odd  $n$  and integer  $k$ . The reason is that

$$\left| g_{k=\frac{\pi n}{N+1}} \left( \frac{N+1}{2} \right) \right| = \left( \frac{2}{N+1} \right)^{1/2} \left| \sin \frac{\pi n}{2} \right| = \begin{cases} 0, & n = 2i, \quad i = 1, 2, \dots \\ \left( \frac{2}{N+1} \right)^{1/2}, & n = 2i + 1, \quad i = 0, 1, \dots \end{cases} \quad (49)$$

For the case  $N = 21$  and  $\beta = 10$  we obtain  $q \approx 0.0061$ . The direct consequence of this property is an equality

$$Q_{(2i_1+1)(2i_1+2l_1+1)} = Q_{(2i_2+1)(2i_2+2l_2+1)}, \quad \forall i_1, i_2, l_1, l_2. \quad (50)$$

Eq.(50) means that we have the system of fermions (the odd nodes) with equal discords between any two of them. This system is a good candidate for the quantum register.

3. If  $j = 1$ , then the profile of the discord  $Q_{n(n+l)}^\beta$ ,  $\forall l$ , is bell-shaped with the maximum  $Q_l^{max}$  in the node  $[\frac{N+1-l}{2}]$  (here  $[a]$  means the integer part of  $a$ ) for discord  $Q_{n(n+l)}^\beta$ . If  $l$  is even, then we have  $g_n(1)|_{n=[\frac{N+1-l}{2}]} = g_{n+l}(1)|_{n=[\frac{N+1-l}{2}]} = \sqrt{\frac{2}{N+1}} \cos \frac{\pi l}{2(N+1)}$  in

eq.(16). If  $l$  is odd, then we have  $g_n(1)|_{n=\lfloor \frac{N+1-l}{2} \rfloor} = \sqrt{\frac{2}{N+1}} \cos \frac{\pi(l+1)}{2(N+1)}$ ,  $g_{n+l}(1)|_{n=\lfloor \frac{N+1-l}{2} \rfloor} = \sqrt{\frac{2}{N+1}} \cos \frac{\pi(l-1)}{2(N+1)}$  in eq.(16). In our example ( $\beta = 10$ ,  $N = 21$ ) we have  $Q_1^{max} \approx 0.0059$ ,  $Q_2^{max} \approx 0.0058$ ,  $Q_3^{max} \approx 0.0055$ ,  $Q_4^{max} \approx 0.0051$ . It is remarkable that  $Q_{n(n+l)} \neq 0$  for all possible  $n$  and  $l$ , i.e. all nodes are correlated. This is a principal advantage of the case  $j = 1$  in comparison with  $j > 1$ , when the discord between some nodes is zero, see Fig.2)

Finally remark, that the unitary invariant discord  $Q_{n(n+l)}^G$  [24] as a function of the node  $n$  for any fixed  $l$  reproduces the shape of  $Q_{n(n+l)}^\beta$  if  $j = 1$  and 11, but  $Q^G$  is bigger than  $Q^\beta$ . Thus, if  $j = 1$ , then  $Q_{n(n+l)}^G$  is bell-shaped with the maximal values  $Q_{max}^G$  equal 0.0108, 0.0106, 0.0099, 0.0093 for  $l = 1, 2, 3, 4$  respectively; if  $j = 11$  and  $l$  is odd, then the unitary invariant discord is the same between any neighbors,  $Q_{n(n+l)}^G \approx 0.0028$ ; if  $j = 11$  and  $l$  is even, then the unitary invariant discord is saw-shaped with the amplitude 0.0110.

## B. Discord and concurrence in a system of $c$ -fermions

Now we consider the  $c$ -representation of the density matrix (see Sec.II B) and calculate the discord and the concurrence between the  $n$ th and  $m$ th  $c$ -fermions. In this case the  $\beta$ -dependence ( $\beta = \frac{\hbar\omega_0}{kT}$ ) of the discord is similar to that given in Fig.2 and it will not be discussed here. Now the entanglement is non-zero for any  $N$  (unlike the entanglement between the  $\beta$ -fermions). Both the discord and the concurrence evolve in time. This evolution for  $\beta = 10$ ,  $N = 21$  and different initially polarized nodes  $j = 1, 6, 11$  is shown in Fig.3 (the discord  $Q_{n(n+1)}^c$  and the concurrence  $C_{n(n+1)}^c$  between the nearest neighbors) and in Fig.4 (the discord  $Q_{n(n+2)}^c$ ). Emphasize the principal differences between the discord and the concurrence.

1. The concurrence is not zero only between the nearest neighbors (except for the concurrence  $C_{13}^c$ , which is not zero in the case of the second initially polarized node,  $j = 2$ ; this concurrence is not shown in Fig.3), while the discord between any two nodes is not identical to zero. For instance, the discord  $Q_{n,n+2}^c$  is shown in Fig.4.
2. The concurrence is not zero only between the neighbors which are closely situated with respect to the initially polarized node. Thus, if  $j = 1$ , then  $C_{12}^c$ ,  $C_{23}^c$  and  $C_{34}^c$  are nonzero; if  $j = 6, 11$ , then only two concurrences (namely,  $C_{j,j\pm 1}^c$ ) are non-zero.

3. After the discord  $Q_{nm}^c$  disappears, it appears again at larger times, see Fig.3, unlike the concurrence which does not appear again. We may refer to this phenomenon as the "echo" in the evolution of the discord, see Fig.3a-c (where the "echo" in evolution of the discord  $Q_{n(n+1)}^c$  is shown for different initially polarized nodes ( $j = 1, 6, 11$ )) and Fig.4 (where the "echo" in evolution of the discord  $Q_{n(n+2)}^c$  is shown). This phenomenon is not observed for the concurrence.
4. Figs.3a-c and 4 demonstrate that the discords  $Q_{n(n+l)}$  and  $Q_{(n+1)(n+l+1)}$  are both non-zero over some common time interval, which is not observed for the concurrence, see Fig.3d-f. This is especially evident for the short time intervals,  $t \lesssim 10$ . This property of the discord might be used, for instance, to organize the relay of the quantum discord from the given pair of nodes to the neighboring pair and so on.

### C. Discord and concurrence in a system of spin-1/2 particles

Now we consider the basis of eigenvectors of the operators  $I_{jz}$  and study the quantum correlations between the  $n$ th and  $m$ th spins (see Sec.II C for the reduced density matrix representation). In this case the concurrence is non-zero and both the discord and the concurrence evolve in time. Emphasize that both the concurrence and the discord are non-zero only between the nearest neighbors (because the discord and the concurrence in the system with the diagonal density matrix are zero and  $\rho_{nm}^{spin}$  is non-diagonal only if  $m = n + 1$ , see Sec.II C). Moreover, since the reduced density matrix for the nearest neighbors coincides with that for the  $c$ -representation (see Sec.II C), both the discord and the concurrence coincide with those obtained in Sec.IV B, i.e  $Q_{n,n+1}^{spin} = Q_{n,n+1}^c$  and  $C_{n,n+1}^{spin} = C_{n,n+1}^c$ , see Fig.3. The basic features of the quantum correlations are following.

1. Similar to the  $c$ -representation, the concurrence is non-zero only between the neighbors which are closely situated to the initially polarized node. Thus, if  $j = 1$ , then  $C_{12}$ ,  $C_{23}$  and  $C_{34}$  are nonzero; if  $j = 6, 11$ , then only two concurrences (namely,  $C_{j,j\pm 1}$ ) are not zero.
2. Similar to Sec.IV B, there is so-called "echo" in the evolution of the discord, while this phenomenon is not observed for the concurrence, see Fig.3.



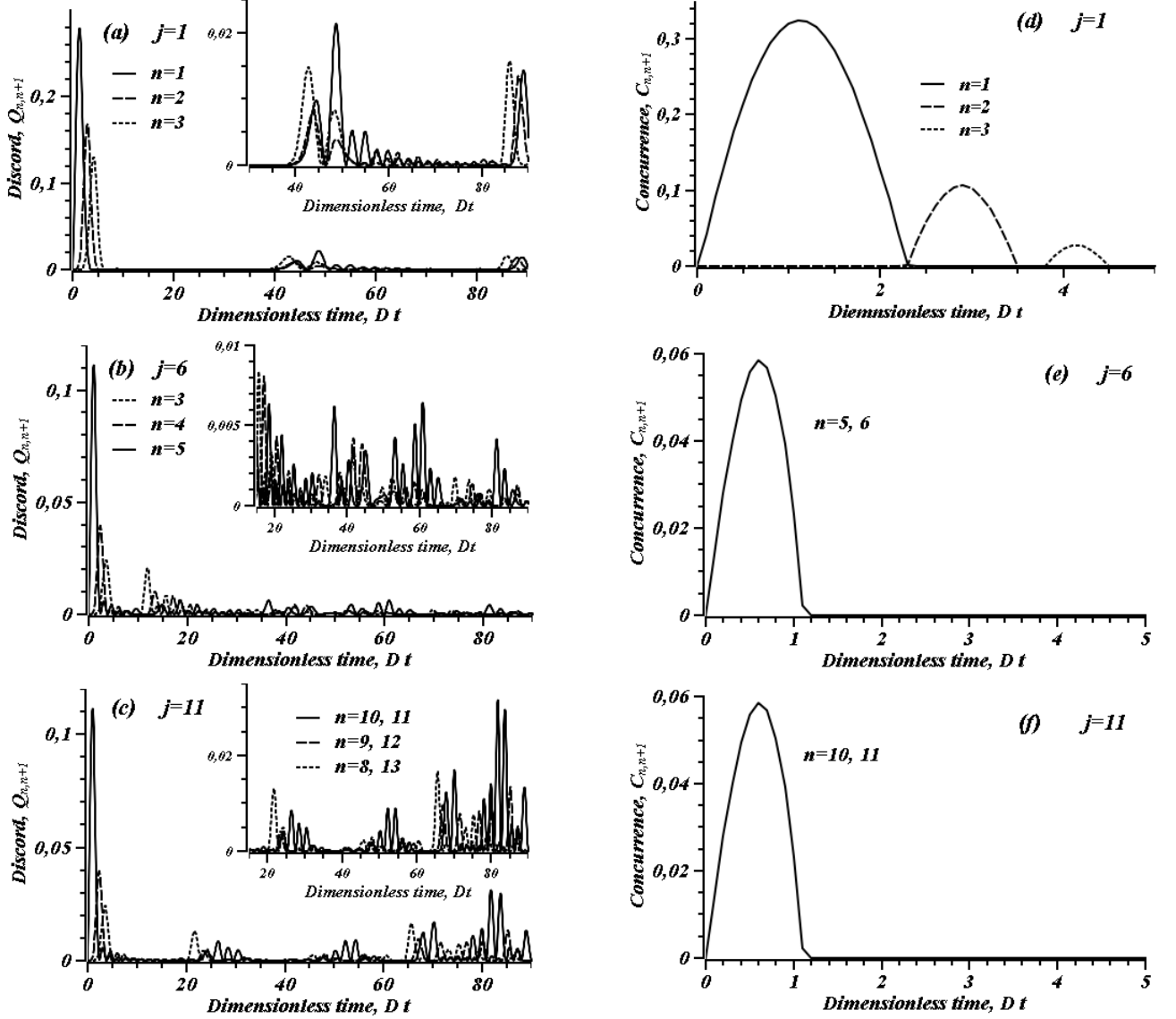


FIG. 3: The time evolution of the discord  $Q_{n,n+1}^c$  (a – c) and the concurrence  $C_{n,n+1}^c$  (d – f) for  $N = 21$  and different initially polarized nodes  $j = 1, 6, 11$ . The insets illustrate the "echo" in the evolution of quantum discord

3. A principal disadvantage of this matrix representation in comparison with the  $c$ -representation is the zero discord between remote nodes.

## V. CONCLUSIONS

For the spin-1/2 open chain of  $N \gtrsim 10$  nodes with the XY Hamiltonian we demonstrate that the behavior of the quantum correlations crucially depends on the basis where these cor-

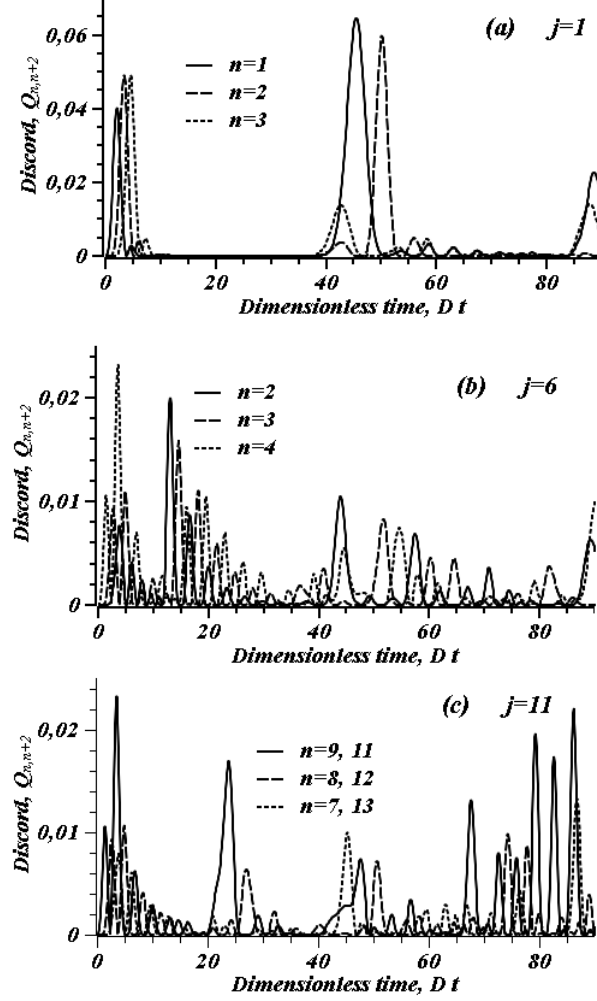


FIG. 4: The time evolution of the discord  $Q_{n,n+2}$  for  $N = 21$  and different initially polarized nodes  $j = 1, 6, 11$

relations are calculated. Thus, both the discord and the concurrence in the  $\beta$ -representation do not evolve in time and concurrence is zero in this case. It is remarkable that the discord is nonzero for the  $\beta$ -representation reflecting the quantumness of the system. It is shown that the system of  $\beta$ -fermions with the middle initially excited node possesses the subsystem of nodes with all equal pairwise discords (the system of odd nodes). If the first node is initially excited, then all nodes are correlated, but the measure of correlations (discord) is different (but non-zero) for each particular pair.

The behavior of the discord and the concurrence in another fermion representation (the  $c$ -representation) significantly differs from their behavior in the  $\beta$ -representation. Both the discord and the concurrence evolve in time, but the concurrence is nonzero only between

the nearest neighbors (there is the single exception for  $C_{23}^c$  in the chain with the second initially polarized node), unlike the discord. In addition, the "echo" is observed in the discord evolution, i.e. after the discord  $Q_{n,m}$  (with any  $m > n$ ) disappears, it appears again at larger times. In this representation we observe the relay of discord from the first pair of the neighboring nodes to the next pair and so on.

Finally, the behavior of the concurrence between the nearest neighbors in the basis of eigenvalues of the operators  $I_{jz}$  coincides with that for the  $c$ -representation. The discord in this basis coincides with the discord in the system of  $c$ -fermions only for the nearest neighbors and equals zero (along with the concurrence) between the remote nodes (i.e.  $m > n + 1$ ).

The proposed analysis of the quantum correlations shows that the representation of a quantum system in the basis of eigenvalues of the operators  $I_{jz}$  is less applicable in quantum devices in comparison with both fermion representations. Since the  $\beta$ - and  $c$ -representations exhibit more variety of quantum correlations, it is more profitable to use the fermions (instead of the real spin-1/2 particles) as nodes in quantum devices. This example demonstrates that the "virtual particles" may reveal some hidden useful properties of a given quantum system.

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